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BU-1106-MA

December 1990  
Revised June 1991

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Abstract

Sexually-transmitted diseases such as gonorrhea, syphilis, herpes, and AIDS are driven and maintained in populations by epidemiological and sociological factors that are not completely understood. One such factor is the way in which people mix sexually. In this paper, we outline a unified approach to modeling sexual mixing structures, where such structures are defined in terms of a set of axioms for a finite number of distinct groups of people. Theorems for homosexual, heterosexual, and arbitrary-group mixing are presented, leading to a representation of all mixing structures defined by the axioms. The representation and its parameters are interpreted in terms of inter-group affinities for sexual mixing. The use of the approach in sexually transmitted disease modeling is discussed.

## 1. INTRODUCTION.

Recent advances in modeling the epidemiology of sexually-transmitted diseases (STDs), and in particular the human immunodeficiency virus (HIV, the causative agent of AIDS), have produced some significant new results in the mathematical description of sexual mixing processes. STD models with more than one group require that a description of sexual mixing among these groups be specified, and there has been considerable attention paid to obtaining a variety of alternative mathematical functions which can provide such a description. In addition to the well-known “proportionate” mixing, *e.g.* [1,4,7,18,20-22,26,39], a version of the assortative mating structure familiar to population geneticists [38] has been used in the STD literature (where it is called “preferred mixing”; *e.g.* [26,29,39]), models with rule-based adaptive sexual behavior have been suggested [3,24], and a number of new “mixing functions” have recently been proposed, *e.g.* [8,15,27-30,34,35,46,47].

Another approach has been to try to deal with mixing functions (a set of functions describing the apportioning of sexual partnerships among groups within a population) in as general a manner as possible. Busenberg and Castillo-Chavez [13,14] generalized the specific case of “like-with-like mixing” [8,9,15], and obtained a representation theorem stating that all mixing functions may be expressed in a special form. Theorems for one- and two-sex populations, with and without age-structure, have been obtained [16], as well as solutions for arbitrarily connected groups of any type [5]. The main advantage of having a representation for mixing is that the effects of wide classes of mixing structure can, in principle, be examined as part of the analysis of a given STD model. A particular case must still be chosen for the purposes of applying such a model to a given situation, but the analysis of the representation would permit such a choice to be made without the danger

that the particular case is in some way special, so that the analysis will include a range of alternative mixing functions.

In this paper we draw together the existing results on representations of mixing and present some new ones with the aim of providing a unified approach to modeling sexual mixing structures for populations composed of a finite number of discrete groups. We present the key theorem of Busenberg and Castillo-Chavez [16] on two-sex models, a new form of the one-sex result, and a new formal derivation of the general case where groups are arbitrary and arbitrarily connected. We discuss the uses of these representations, the interpretation of their parameters, and address the requirements which must be met for the implementation of particular cases in STD models.

## 2. MIXING REPRESENTATIONS.

A number of results on the representation of sexual mixing processes have now been developed [5,13,14,16], which we will summarize and expand upon in this section. In each case, we present a brief statement of the problem, and derive a representation of solutions to that problem. In the subsequent section we consider the interpretation of the parameters of the representation.

### 2.1 The one-sex case, with $N$ active groups.

We consider mixing in a population comprised of  $N$  distinct groups, in the  $i^{\text{th}}$  of which there are  $T_i(t)$  individuals with average activity (defined as the number of partners taken per unit time)

$C_i(t)$ , at time  $t$ . Here we assume that  $C_i(t) \gg 0$  and  $T_i(t) \gg 0$  for all  $t$ , that is, *all individuals in each group have some strict positive level of sexual activity, no group ever becomes empty, and some degree of mixing may occur between any pair of groups, including self-mixing*. The usual approach to modeling the mixing process (who has sex with whom) may conveniently be expressed in terms of an  $N \times N$  matrix  $\mathbf{p}(t)$ , where  $p_{ij}(t)$  is the average fraction of the partners of a person in group  $i \in [1, N]$  coming from group  $j \in [1, N]$ , at time  $t$ , given that they have sex. Any such  $\mathbf{p}$ , a conditional probability distribution, must satisfy the following constraints:

$$0 < p_{ij}(t) < 1 \quad , \text{ all } i, j \text{ and } t, \quad (1)$$

$$\sum_{j=1}^N p_{ij}(t) = 1 \quad , \text{ all } i \text{ and } t, \quad (2)$$

$$C_i(t) T_i(t) p_{ij}(t) = C_j(t) T_j(t) p_{ji}(t) \quad , \text{ all } i, j \text{ and } t. \quad (3)$$

Constraints (1) and (2) simply make  $\mathbf{p}$  a stochastic matrix (the strict inequalities in (1) arising because in this section we do not permit a complete lack of mixing between any pair of groups), and (3) enforces conservation of the number of new pairings per unit time between individuals in groups, given that they have sex.

**Theorem 1.** All  $\mathbf{p}$  satisfying (1) – (3) for all time  $t$  may be written, in terms of a nonnegative symmetric matrix  $\Phi(t) = (\phi_{ij}(t))$ , as follows:

$$p_{ij}(t) = \bar{p}_j(t) \left[ \frac{R_i(t) R_j(t)}{V(t)} + \phi_{ij}(t) \right] \quad , \text{ all } i, j, t, \quad (4)$$

where

$$R_i(t) = 1 - \sum_{k=1}^N \bar{p}_k(t) \phi_{ik}(t) \geq 0 \quad , \text{ all } i \quad (5)$$

$$V(t) = \sum_{k=1}^N \bar{p}_k(t) R_k(t) \quad , \quad (6)$$

and

$$\bar{p}_j(t) \equiv \frac{C_j(t) T_j(t)}{\sum_{k=1}^N C_k(t) T_k(t)} \quad , \text{ all } j. \quad (7)$$

$\bar{p}_j$  is the average fraction of the total activity in the population due to group  $i$ , and  $p = \bar{p}$  is a solution to the axiomatic system (1)–(3), known as proportionate mixing, and results when a “typical” group individual mixes at random (mixing of typical individuals is weighed by the average sexual activity of their corresponding group.) An outline of an alternative proof, to this theorem of Busenberg and Castillo-Chavez [14], is provided below.

Outline of Proof Define  $\Psi_{ij} \equiv p_{ij} / \bar{p}_j$ , a set of functions which are strictly positive and finite for the problem as stated, and which from (3) are jointly symmetric,  $\Psi_{ji} = \Psi_{ij}$  all  $i$  and  $j$ . We look for a representation containing  $\Psi$  of the form

$$\Psi_{ij} = \Omega_i \Omega_j + \phi_{ij} \quad , \quad (8)$$

where  $\Omega$  is a vector of  $N$  functions, such that all products  $\Omega_i \Omega_j$  are real and positive, and  $\phi$  is an  $N \times N$  matrix where  $\phi_{ji} = \phi_{ij}$  is required to maintain the symmetry imposed on  $\Psi$  by (3). The  $\Omega_i \Omega_j$  act as “reference surface”, as yet unspecified, and the  $\phi$  are the deviations from  $\Psi$ . Multiplying through (8) by  $\bar{p}_j$  and summing over all  $j$  gives the implicit relation for each  $\Omega_i$ ,

$$\Omega_i = \frac{1 - \sum_{k=1}^N \bar{p}_k \phi_{ik}}{\sum_{k=1}^N \bar{p}_k \Omega_k}. \quad (9)$$

Multiplying through by  $\bar{p}_i$ , and summing over all  $i$ , yields (because the  $\bar{p}_j$  sum to unity, Eq (7))

$$\sum_{k=1}^N \bar{p}_k \Omega_k = \left[ \sum_{k=1}^N \bar{p}_k \left\{ 1 - \sum_{l=1}^N \bar{p}_l \phi_{kl} \right\} \right]^{\frac{1}{2}}. \quad (10)$$

Substituting (9) and (10) into (8), and recalling the definition of  $\Psi$ , allows us to write all  $p$  satisfying Eqs (1) – (3) in the form (4), with  $R_i$  and  $V$  as defined in (5) and (6).

We have included the time argument  $t$  in Eqs (4) – (6) to emphasize that  $p(t)$  must be valid for all time  $t$ , and that the elements of  $\phi$  may be implicit through the elements of  $p(t)$  or explicit functions of time. In Section 3 we consider the interpretation of the quantities  $\phi$ .

## 2.2 The two-sex case, with all groups active.

We start by defining a set of mixing functions  $\{p_{ij}^m(t)\}$  and  $\{p_{ji}^f(t)\}$ , with  $i \in [1, N^m]$  ( $N^m$  the number of male sub-groups), and  $j \in [1, N^f]$  ( $N^f$  the number of female sub-groups). We have  $p_{ij}^m(t)$ ,



the proportion of partnerships of males in group  $i$  with females in group  $j$ , and  $p_{ji}^f(t)$ , the proportion of partnerships of females in group  $j$  with males in group  $i$ , at time  $t$ . Also we let  $C_i^m(t)$  be the average rate at which males in group  $i$  form partnerships with females, and  $C_j^f(t)$  the average rate at which females in group  $j$  form partnerships with males. Here we have  $T_i^m(t)$ , the number of males in group  $i$ , and  $T_j^f(t)$ , the number of females in group  $j$ , at time  $t$ . We relax the strict assumption of the previous sub-section, and include the case where  $T_j^f(t)$ ,  $T_i^m(t)$ ,  $C_j^f(t)$  and  $C_i^m(t)$  may become zero for some  $t$ .

The  $p_{ij}^m$  and  $p_{ji}^f$  must satisfy a set of constraints, related to Eqs (1) – (3); specifically, for  $(p_{ij}^m, p_{ji}^f)$  to be a mixing matrix, it must satisfy the following properties at all times:

$$0 \leq p_{ij}^m \leq 1, \quad 0 \leq p_{ji}^f \leq 1, \quad (11)$$

$$\sum_{j=1}^{N^f} p_{ij}^m = \sum_{i=1}^{N^m} p_{ji}^f = 1, \quad (12)$$

$$C_i^m T_i^m p_{ij}^m = C_j^f T_j^f p_{ji}^f, \quad i = 1, \dots, N^m, \quad j = 1, \dots, N^f. \quad (13)$$

Also, if for some  $i$ ,  $0 \leq i \leq N^m$  and/or some  $j$ ,  $0 \leq j \leq N^f$ , at any time  $t$ , we have that

$$C_i^m(t) C_j^f(t) T_i^m(t) T_j^f(t) = 0, \quad (14)$$

then we define

$$p_{ij}^m(t) \equiv p_{ji}^f(t) \equiv 0. \quad (15)$$

Eq (14) can be viewed as a conservation law for the rates of partnership formation, while Eq (15) asserts that the mixing of “non-existing” or non-sexually active sub-populations does not occur. We now define the quantities

$$\bar{p}_j^m \equiv \frac{C_j^f T_j^f}{\sum_{k=1}^{N^m} C_k^m T_k^m} \quad (16)$$

and

$$\bar{p}_i^f \equiv \frac{C_i^m T_i^m}{\sum_{k=1}^{N^f} C_k^f T_k^f}, \quad (17)$$

for  $j = 1, \dots, N^f$  and  $i = 1, \dots, N^m$ , as special two-sex mixing solutions which correspond to purely heterosexual proportionate or random mixing. The following result was established recently by Castillo-Chavez and Busenberg [16]:

*Theorem 2.* Let  $\{\phi_{ij}^m(t)\}$  and  $\{\phi_{ji}^f(t)\}$  be two non-negative matrices. Let

$$\ell_i^m \equiv \sum_{k=1}^{N^f} \bar{p}_k^m \phi_{ik}^m \quad (18)$$

and

$$\ell_j^f \equiv \sum_{k=1}^{N^m} \bar{p}_k^f \phi_{jk}^f, \quad (19)$$

where  $\{(\bar{p}_j^m, \bar{p}_i^f), j = 1, \dots, N^f \text{ and } i = 1, \dots, N^m\}$  denotes the set of Ross<sup>1</sup> solutions. We also let  $R_i^m \equiv 1 - \ell_i^m$ ,  $i = 1, \dots, N^m$  and  $R_j^f \equiv 1 - \ell_j^f$ ,  $j = 1, \dots, N^f$ , and assume that  $\phi_{ij}^m$  and  $\phi_{ji}^f$  are chosen in such a way that  $R_i^m$  and  $R_j^f$  remain non-negative for all time. We further assume that

$$\sum_{i=1}^{N^m} \ell_i^m \bar{p}_i^m = \sum_{i=1}^{N^m} \sum_{k=1}^{N^f} \bar{p}_k^m \phi_{ik}^m \bar{p}_i^m < 1,$$

and

$$\sum_{j=1}^{N^f} \ell_j^f \bar{p}_j^f = \sum_{j=1}^{N^f} \sum_{k=1}^{N^m} \bar{p}_k^f \phi_{jk}^f \bar{p}_j^f < 1 .$$

Then all the solutions to the axiom Eqs (11) – (15) are given by

$$p_{ij}^m = \bar{p}_j^m \left[ \frac{R_j^f R_i^m}{\sum_{k=1}^{N^f} \bar{p}_k^m R_k^f} + \phi_{ij}^m \right] \quad (20)$$

and

$$p_{ji}^f = \bar{p}_i^f \left[ \frac{R_i^m R_j^f}{\sum_{k=1}^{N^m} \bar{p}_k^f R_k^m} + \phi_{ji}^f \right] \quad (21)$$

for  $i = 1, \dots, N^m$  and  $j = 1, \dots, N^f$ . Thus Eqs (20) – (21) provide a way of representing all two-sex

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<sup>1</sup>The search for “separable” solutions to Eqs (20) and (21), that is, solutions where  $p_{ij}^m = \omega_i \omega_j'$  and  $p_{ji}^f = \eta_j \eta_i'$  for some appropriate functions  $\{\omega_i\}$ ,  $\{\omega_i'\}$ ,  $\{\eta_i\}$  and  $\{\eta_i'\}$ , leads to (see [16]) the unique solution  $p_{ij}^m = \bar{p}_j^m$  and  $p_{ji}^f = \bar{p}_i^f$ . Eqs (15) and (16) are the only separable solutions to the two-sex mixing problem; this result is a direct consequence of (13). Ross in 1911 [44] was the first to write down the requirement that the number of interactions must be conserved (*op. cit.* p 667); here explicitly given as a constraint (see Eq (3)). He was motivated by malaria transmission models, but wrote in a wider context of interactive events (“Happenings and Becomings”, p 655), and explicitly recognized that STDs could be modeled in a two-sex population in essentially the same way (p 685). He did not restrict his consideration to cases where the total population was constant (p 678). Much of his work was reported by Lotka [96], including the point about conservation of interactions (*e.g.* p 305). Ross’ contributions to STD applications have not been widely recognized. The solutions given by Eqs (15) and (16) are based on ratios of male to female sexual activity and are equivalent to the mixing ratios of vector to host-biting activity given by Ross (he only considered two groups). Consequently, we refer to Eqs (15) and (16) as the *Ross solutions* to the two-sex mixing problem (see also [13,14,16]); as they do not themselves involve the  $\phi^f$  and  $\phi^m$ , there should be no confusion over this terminology. Furthermore, we observe that if  $\phi_{ij}^f \equiv a$  and  $\phi_{ij}^m \equiv b$  for all  $i$  and  $j$ ,  $a$  and  $b$  constants, Eqs (20) and (21) reduce to the Ross solutions. This corresponds to the situation in which males and females do not exhibit group-specific affinities

mixing problems when specified in the form of the constraints, Eqs (11) – (15).

Returning to the general solution to the two-sex case, it is important to note that (18) – (21) are not automatically satisfied for arbitrary  $T_j^f(t)$ ,  $T_i^m(t)$ ,  $C_j^f(t)$  and  $C_i^m(t)$ . This reflects a well-known observation in the demographic literature, that the two-sex problem has no unique solution [23,32,37,42,43], in that all of the  $C$  cannot remain fixed for all time; pair-formation functions [13,17,20-23,42] represent an example of how male and/or female activity levels may be adjusted so as to satisfy the mixing constraints. Substituting (16), (17) (20) and (21) back into (13) (the conservation of partnerships constraint), we see that the equality

$$\frac{\sum_{k=1}^{N^f} C_k^f T_k^f}{\sum_{k=1}^{N^m} C_k^m T_k^m} = 1 = \frac{\left[ \frac{R_j^f R_i^m}{\sum_{k=1}^{N^f} \bar{p}_k^m R_k^f} + \phi_{ij}^m \right]}{\left[ \frac{R_i^m R_j^f}{\sum_{k=1}^{N^m} \bar{p}_k^f R_k^m} + \phi_{ji}^f \right]} \quad (22)$$

must be satisfied at all time  $t$ , because

$$\sum_{k=1}^{N^f} C_k^f(t) T_k^f(t) = \sum_{k=1}^{N^m} C_k^m(t) T_k^m(t) \equiv Q(t) \quad (23)$$

must hold true, as a consequence of constraint (13).

Even with  $\phi_{ji}^f = \phi_{ij}^m$ , Eq (23) is not guaranteed, however, as in principle all the quantities  $T_j^f(t)$ ,  $T_i^m(t)$ ,  $C_j^f(t)$  and  $C_i^m(t)$  are free to vary within the STD model in which the description of mixing is

embedded. In a given model, we have to make sure that (23) is not violated, for example by providing rules for calculating some sub-set of the male or female activity levels at every time  $t$ , effectively incorporating (23) directly into the model [9,17] (alternatively, there may be in some cases ways of satisfying (22) by adjusting the  $\phi$  for males or females at each time  $t$  during a realization of the STD model). In the appendix we give an example of a pair-formation model of gonorrhea transmission in a multi-group two-sex population complete with specified  $\phi$  and rules for adjusting the  $C_j^f(t)$  and  $C_i^m(t)$  so as to satisfy (23).

A consequence of (23) is that the denominators in Eqs (16) and (17) are equal, so that the Ross solutions may be written in the form  $(C_j^f T_j^f / Q, C_i^m T_i^m / Q)$ .

### 2.3 Arbitrarily connected groups.

The mixing problem in this general case may be stated as follows. Let there be  $N$  distinct sub-groups within a given population, and let  $i$  ( $i \in \mathcal{K}$ ,  $\mathcal{K} = [1, N] \in \mathcal{N}^+$ ) be an index for the groups. The groups' population sizes and activity levels (number of partnerships formed per unit time) are given respectively by  $T_i(t)$  and  $C_i(t)$  for  $i \in \mathcal{K}$ , at time  $t$ . Let  $p_{ij}(t)$  denote the fraction of these partnerships for group  $i$  which are formed with group  $j$  at time  $t$ , given that they have sex. We must deal with two types of zero: those arising when one or more of the quantities  $C_i(t)T_i(t)$  equal zero for some  $t$  (*i.e.* when due to the details of the dynamic model in which the mixing process is embedded, a particular group or groups become inactive or empty), and those due to a fundamental lack of direct connection between two groups (*e.g.* between male and female homosexuals, or the incompleteness of any network of sexual partnerships [33]). For the first of these, we introduce

$\chi_i(C_i(t)T_i(t))$ ,  $i \in \mathfrak{K}$ , characteristic functions such that

$$\chi_i(C_i T_i) = \begin{cases} 1 & , C_i T_i > 0 \\ 0 & , C_i T_i = 0 \end{cases} . \quad (24)$$

For the second (connectedness) zeros, we introduce a second set of characteristic functions,  $\mathfrak{X}_{ij}$  ( $i, j \in \mathfrak{K}$ ), such that

$$\mathfrak{X}_{ij} = \begin{cases} 1 & , \text{groups } i \text{ and } j \text{ connected,} \\ 0 & , \text{groups } i \text{ and } j \text{ not connected.} \end{cases} . \quad (25)$$

We will assume that for each group there is at least one group with which it mixes, *i.e.* every row of the matrix  $\mathfrak{X}$  contains at least one element with value unity. We assume that enough of the  $\{\chi_i\}$  and  $\{\mathfrak{X}_{ij}\}$  are non-zero to make the problem relevant. With this notation the axiomatic constraints on the mixing problem for arbitrarily connected groups, which must be true for all time  $t$ , become

$$\begin{aligned} (i) \quad & 0 \leq p_{ij} \leq 1 , & i, j \in \mathfrak{K} \\ (ii) \quad & \sum_{j \in \mathfrak{K}} \mathfrak{X}_{ij} \chi_i \chi_j p_{ij} = \chi_i , & i \in \mathfrak{K} \\ (iii) \quad & \mathfrak{X}_{ij} \chi_i C_i T_i p_{ij} = \mathfrak{X}_{ji} \chi_j C_j T_j p_{ji} , & i, j \in \mathfrak{K} \end{aligned}$$

where we have dropped the argument of  $\chi_i$  for convenience, and retained  $\mathfrak{X}_{ij} = \mathfrak{X}_{ji}$  on both sides of (iii) for clarity. Constraints (i) and (ii) simply require  $p$  to behave like a conditional probability density function, where it exists, while constraint (iii) enforces the conservation of partnership acquisition rates between active, non-empty, connected groups. We make use of the quantity

$$\bar{P}_j \equiv \frac{\chi_j C_j T_j}{\sum_{k \in \mathfrak{K}} \chi_k C_k T_k} , \quad j \in \mathfrak{K} , \quad (26)$$

the fraction of total activity provided by the  $j^{\text{th}}$  group.

The following discussion brings together the Representation Theorem of Busenberg and Castillo-Chavez [13,14,16], and the less formal results of Blythe [5] on systems with arbitrarily connected groups to show that any solution  $p$  to the axioms (i)–(iv) may be written in a common form. First note that Axiom (iii) may be written

$$\frac{p_{ij}}{p_{ji}} = \frac{\chi_j \mathfrak{X}_{ij} C_j T_j}{\chi_i \mathfrak{X}_{ji} C_i T_i}, \quad i \text{ and } j \in \mathfrak{K} \quad (27)$$

(equal to zero if any of  $\mathfrak{X}_{ij}$ ,  $\chi_i$ ,  $\mathfrak{X}_{ji}$ ,  $\chi_j$  equal zero) suggesting that we deal with the quantities

$$\Psi_{ij} \equiv \frac{p_{ij}}{\bar{p}_j} \mathfrak{X}_{ij} \chi_i \mathfrak{X}_{ji} \chi_j, \quad i, j \in \mathfrak{K} \quad (28)$$

(as in Section 2.1) which exist only where active non-empty groups are connected. By definition the  $\Psi_{ij}$  are finite and non-zero where mixing occurs, zero (undefined) elsewhere, and jointly symmetric:  $\Psi_{ji} = \Psi_{ij}$ ,  $i$  and  $j \in \mathfrak{K}$ . We may choose to write the  $\Psi_{ij}$  in the form

$$\Psi_{ij} = \left( \frac{\Gamma_i \Gamma_j}{\Lambda} + \phi_{ij} \right) \mathfrak{X}_{ij} \chi_i \mathfrak{X}_{ji} \chi_j, \quad i, j \in \mathfrak{K}, \quad (29)$$

that is to say, as a reference surface (the product term) plus whatever is needed give  $\Psi$ . We restrict the products  $\Gamma_i \Gamma_j$ , and the functions  $\phi_{ij}$  to all be real. Axiom (ii) tells us that we may write

$$\sum_{k \in \mathfrak{K}} \bar{p}_k \Psi_{ik} \mathfrak{X}_{ik} \chi_i \mathfrak{X}_{ki} \chi_k = \chi_i, \quad i \in \mathfrak{K}, \quad (30)$$

so applying this to Eq (29) gives us the relations

$$\chi_i = \chi_i \Gamma_i \frac{\sum_{k \in \mathfrak{K}} \chi_k \mathfrak{X}_{ik} \bar{p}_k \Gamma_k}{\Lambda} + \chi_i \sum_{k \in \mathfrak{K}} \chi_k \mathfrak{X}_{ik} \bar{p}_k \phi_{ik}, \quad i \in \mathfrak{K}. \quad (31)$$

We now choose  $\Lambda$  to simplify the problem, at the same time imposing a restriction on  $\bar{p}_k$  and/or  $\phi_{ik}$ . Let

$$\sum_{k \in \mathfrak{K}} \chi_k \mathfrak{X}_{ik} \bar{p}_k \Gamma_k = \Lambda, \quad \text{all } i \in \mathfrak{K}, \quad (32)$$

*i.e.* all the  $N$  quantities on the LHS of Eq (32) must be equal, as they depend on the *fixed* connectedness structure of the population. Then

$$\Gamma_i = 1 - \sum_{k \in \mathcal{K}} \chi_k \mathfrak{X}_{ik} \bar{P}_k \phi_{ik}, \quad i \in \mathcal{K}, \quad (33)$$

and we may write

$$p_{ij}(t) = \chi_i \chi_j \mathfrak{X}_{ij} \bar{P}_j(t) \left[ \frac{\chi_i \Gamma_i(t) \chi_j \Gamma_j(t)}{\Lambda(t)} + \phi_{ij}(t) \right], \quad i \text{ and } j \in \mathcal{K}, \quad (34)$$

*iff* Eq (32) holds. This constraint may be written as the set of  $N - 1$  equations

$$\sum_{k \in \mathcal{K}} (\mathfrak{X}_{ik} - \mathfrak{X}_{jk}) \chi_k \bar{P}_k \left\{ 1 - \sum_{u \in \mathcal{K}} \chi_u \mathfrak{X}_{ku} \bar{P}_u \phi_{ku} \right\} = 0, \quad i \text{ and } j \in \mathcal{K} \quad (35)$$

which may be cast in the quadratic form

$$\sum_{k, u \in \mathcal{K}} \alpha_{ijk u} y_k y_u = 0, \quad i, j \in \mathcal{K}, \quad (36)$$

where

$$\alpha_{ijk u} \equiv (\mathfrak{X}_{ik} - \mathfrak{X}_{jk}) (1 - \mathfrak{X}_{ku} \phi_{ku}), \quad i, j, k, u \in \mathcal{K}$$

and

$$y_i \equiv \chi_i C_i T_i, \quad i \in \mathcal{K}.$$

Any mixing function which satisfies the mixing axioms ((i) – (iii) in general, or the particular cases (1) – (3) or (11) – (15)) may be written in the form of Eq (34) and (36). This includes all descriptions [17] which do not involve concurrent partnerships, *e.g.* [6, 49].

It has been shown [5] that the problem of satisfying (36) has, under some circumstances, solutions which involve adjusting  $\phi$  alone. Alternatively, we may view Eqs (36) as  $N - 1$  equations in the  $N$  quantities  $C_i$ , at each time  $t$ , so that in principle a solution can always be obtained by adjusting the  $C_i$  (in fact we can expect either zero or an infinite number of such solutions). Trivially,  $C_i(t) = 0$  ( $i \in \mathcal{K}$ , all  $t$ ) is always a solution. When all groups are connected ( $\mathfrak{X}_{ij} = 1$ ,  $i, j \in \mathcal{K}$ ), and  $\chi_i = 1$  ( $i \in \mathcal{K}$ ), then Eqs (36) are always satisfied. For a strictly two-sex model, with each male (female) group connected to all female (male) groups, but not to any of their own sex, then Eqs (36) reduce to the requirement that the total rate of partnership formation in males equals that in females. Eq (23) can be achieved by alteration of the group activity levels  $C_i(t)$ , [2, 3, 20, 21, 24, 25, and the



appendix]. In the arbitrarily connected case, special solutions can exist where (36) is satisfied by making some of the  $\phi$  adjust [5], but it will usually be necessary to alter some or all of the  $C_i$ . The crucial feature of a population sub-divided into  $N$  groups is the number of “self-loops”, *i.e.* the number of groups where  $\mathfrak{X}_{ii} = 1$ , so that individuals may take partners from the home group [5]. If there are  $N$  self-loops, then a solution may always be found where the  $C_i$  need not be adjusted (the proof of this is trivial: if there are *only* self-loops a solution always exists). In Section 3 we return to the idea of adjusting the  $C_i(t)$ .

That some or all of the  $C$  or  $\phi$  are not free to take arbitrary values so that Eqs (36) are satisfied represents a restriction, but a completely realistic one. If noone in the population *completely* discounts anyone else as a potential partner, then everyone can get as many partners as they wish, regardless of how low or high a number that may be. When some connections are forbidden, *i.e.* some groups never mix, then in at least some of the groups either preference must change if a target activity is to be met (although there are limits as to how much adjustment is possible [5]), or the target activity must change.

If sexual activity  $C$  represents a continuum in the population, rather than being given for discrete groups, then the characteristic functions  $\mathfrak{X}$  must be defined with respect to the subset of  $(C, C')$  which can interact; the counterpart of adjusting the  $C_i(t)$  in this case is the manipulation of the density function of individuals with activity  $C$  in the population. If age further characterizes the population and the mixing process, then we must similarly use appropriate characteristic functions [14,15,19] to allow “unconnected” age ranges. Eq (11) has applications in many areas as a general representation of paired-event processes [10], and may be generalized for an arbitrary number of dimensions [11].

Strictly speaking, there are no truly separable solutions to the arbitrary connected case such as the Ross solutions of Section 2.2 because the connectedness indicator functions  $\{\mathfrak{X}_{ij}\}$  are involved in all pair-wise interactions. However we may find solutions which are separable, *conditional* upon connectance.

**Theorem 3.** For a population where the graph of  $\mathfrak{X}$  contains no disjoint sub-sets, the mixing function  $p_{ij} = \chi_i \chi_j \mathfrak{X}_{ij} C_j T_j / D_i$ , for  $D_i \equiv \sum_{k \in \mathfrak{K}} \mathfrak{X}_{ik} \chi_k C_k T_k = \mathfrak{R} > 0$ , for all  $i \in \mathfrak{K}$ , gives the only conditional separable solution of Eq (34).

Proof. Let  $p_{ij} = \chi_i \omega_i \chi_j \omega'_j \mathfrak{X}_{ij}$ , for some non-negative functions  $\{\omega_i, \omega'_j\}$ . Summing over all  $j$ , and using (iii), we have  $\chi_i \omega_i K_i = \chi_i$ , where

$$K_i \equiv \sum_{k \in \mathfrak{K}} \mathfrak{X}_{ik} \chi_k \omega'_k > 0,$$

so that

$$p_{ij} = \mathfrak{X}_{ij} \chi_i \chi_j \frac{\omega'_k}{K_i}.$$

Substituting into (iii) to get

$$\mathfrak{X}_{ij} \chi_i \chi_j C_i T_i p_{ij} = \mathfrak{X}_{ij} \chi_i \chi_j C_j T_j \frac{\omega'_i}{K_j},$$

and summing over all  $j$ , we have  $\chi_i C_i T_i = \chi_i \omega'_i Q_i$  where

$$Q_i \equiv \sum_{k \in \mathfrak{K}} \mathfrak{X}_{ik} \chi_k \frac{C_k T_k}{K_k}.$$

Then from (iii) we require  $K_i Q_j = K_j Q_i$ , for all  $i$  and  $j$  (by the hypothesis of the theorem, there are no disjoint sub-sets of  $i$  and  $j$ ), so that  $K Q$  must equal a constant  $\mathfrak{R}$ , and  $p_{ij} = \chi_i \chi_j \mathfrak{X}_{ij} C_j T_j / \mathfrak{R}$ . But the  $p_{ij}$  must sum to  $\chi_i$  over  $j$  for each  $i$ , so that

$$D_i \equiv \sum_{k \in \mathfrak{K}} \mathfrak{X}_{ik} \chi_k C_k T_k = \mathfrak{R} > 0.$$

The equivalent form of Eq (36) must be satisfied for some  $D$  and all  $i$  for a separable solution to exist, and the proof is complete. Both proportionate mixing in the one-sex case (Section 2.1) and the Ross solutions in the two-sex case (Section 2.2) may be recovered with appropriate choices of  $\mathfrak{X}$ . Again, some or all of the  $C$  may need to be adjusted at each time  $t$  in order to satisfy the constraints.

The arbitrary-connections case Eq (32) may be used to generate all particular cases of  $N$ -group mixing. For example, one may set all the elements of  $\chi$  and  $\mathfrak{X}$  equal to unity, and recover the formulation of Section 2.1. The two-sex result of Section 2.2 may be obtained by noting that  $\mathfrak{R} = 2\mathfrak{G}$ ,

introducing an appropriate ordering of the  $\{i\}$  for the two sexes with  $\mathfrak{X}$  a block matrix, and writing  $\phi_{uv}^f = \phi_{vu}^m = \frac{1}{2}\phi_{ij} = \frac{1}{2}\phi_{ji}$  ( $u$  and  $v$  appropriately chosen indices). The definition of “groups” can be extremely broad; for example, one can use groups defined by geographical location, sexual orientation, disease status [41], or gender.

In this section we have considered three variants of the representation of  $p$ . In 2.1 we derived a representation when all  $N$  groups are connected to each other (partners may come from anywhere), and in no group does the total activity  $C_i T_i$  ever equal zero. Then the representation is unconstrained; it is enough to specify the  $\phi$  due to the presence of self-loops in all groups. In 2.2 we dealt with the two-sex problem, showing that the representation then includes a constraint which must be satisfied at all time  $t$ . This may be achieved by adjusting the activity levels  $C^f$  and/or  $C^m$ . In 2.3 we discussed the full form of the representation, where the  $N$  groups are arbitrarily connected, and some of the quantities  $C_i T_i$  may be zero for some  $t$ . There can be solutions with variable  $\phi$ , and there are always solutions where some or all of the  $C$  are adjusted. In this paper we do not discuss the details of the two types of solutions  $\phi$ -adjusted and  $C$ -adjusted; an example of the latter may however be found in the appendix for the two-sex case.

### 3. INTERPRETING THE $\phi$ .

In the previous section it was shown that in the general case of the representation, a set of constraints (36) must be satisfied for a solution (34) to hold. Some solutions may be found by adjusting the  $\phi$  at every time-step in a dynamic model, but we may always find solutions by adjusting the  $C$  (and leaving the  $\phi$  as defined parameters or functions). In the light of this observation, it is tempting to interpret the  $\phi$  as structural quantities, defining the way in which partnerships are allocated among groups subject to demand and supply,  $C$ . As there is one  $\phi_{ij} = \phi_{ji}$  for each pair-wise interaction among groups (including possible interactions of a group with itself), we might extend the structural interpretation to one of inter-group affinity or preference.

### 3.1 The $\phi$ as affinities.

Consider the special case of Section 2.1, where all groups interact. If all the products  $C_i T_i$  are equal (all groups have equal total activity), then the mixing from Eq (8) is given by

$$p_{ij} = \frac{1}{N} \left[ \phi_{ij} + \frac{(1 - \bar{\phi}_i)(1 - \bar{\phi}_j)}{(1 - \bar{\phi})} \right], \quad (37)$$

where

$$\bar{\phi}_i = \frac{1}{N} \sum_{j=1}^N \phi_{ij}$$

and

$$\bar{\phi} = \frac{1}{N} \sum_{i=1}^N \bar{\phi}_i .$$

In Eq (37), if we associate a number between zero and unity with each pair-wise intergroup interaction, then we obtain a mixing function satisfying the axioms. It is tempting to interpret the  $\phi$  as structural parameters, reflecting some sort of affinity between each pair of groups, for in the absence of any other differences between groups the  $\phi$  specify the pattern of non-random mixing. The  $\phi$  interact in Eq (37); the absolute magnitude of each  $\phi_{ij}$  has a direct effect, but so do the relative magnitudes of the *averages* of  $\phi$  in the  $i^{\text{th}}$  and in the  $j^{\text{th}}$  groups with respect to the overall average of  $\phi$ . This is not incompatible with the interpretation that the  $\phi$  may be regarded as intergroup affinities, as the *net* effect of a variety of affinity structures may in some cases be the same. This is very clearly the case where all the  $\phi$  are equal to a constant (say  $\theta$ ). Then regardless of the value of  $\theta$ , we always have  $p_{ij} = 1/N$ , *i.e.* a special case of proportionate mixing, when all  $C_i T_i$  are equal. In fact, if  $\phi_{ij} = 1 - \theta_i \theta_j$  (where the  $\theta$  are any real functions such that  $\theta_i < 1$ , all  $i$ ), then proportionate mixing results, indicating that the appearance of randomness may arise from a very wide variety of structures. The calculation of each  $p_{ij}$  involves all of the  $\phi$ .

We suggest that any definition of affinity must include the following properties:

- (a) The affinity between each pair of groups is a unique number, and all such affinities should have independent values;

(b) The overall pattern of mixing in the population is influenced by the affinities, and in the absence of any other differences among the groups, is specified entirely by the affinities;

(c) The size of the affinity numbers should reflect the degree of interaction between the pairs of groups.

There is arguably a fourth criterion for affinity. Ideally, one would think that there should be a well-defined numerical range for the affinities covering the continuum from minimal to maximal mixing, with random (proportional) mixing lying somewhere between these extremes. It is not clear, however, what this range should be, as there are many numerically-based definitions of preference consonant with (a) – (c).

From the preceding discussion, we see at once that  $\phi$  satisfies (a) and (b). To demonstrate that (c) is also satisfied, consider a particular  $\phi_{ij} = \sigma$  in Eq (37). Recalling that  $\phi_{ji} = \phi_{ij}$ , so that both  $\bar{\phi}_i$  and  $\bar{\phi}_j$  depend on  $\sigma$ , then the mixing fraction for this particular  $i$  and  $j$ ,  $p_{ij}$  varies with  $\sigma$  such that

$$\frac{\partial p_{ij}}{\partial \sigma} = \frac{(1 - \bar{\phi}_i(\sigma)) + (1 - \bar{\phi}_j(\sigma))}{N^2(1 - \bar{\phi}(\sigma))} + \frac{2(1 - \bar{\phi}_i(\sigma))(1 - \bar{\phi}_j(\sigma))}{N^3(1 - \bar{\phi}(\sigma))^2}. \quad (38)$$

A sufficient condition for this partial derivative to be positive is that all the elements of  $\{\bar{\phi}_i\}$  have values less than unity, so that the  $\phi$  satisfy the third of our criteria for affinities.

On the basis of the above, we feel that we can interpret the  $\phi$  as affinities between groups. The ranges of values of  $\phi$ , and whether they are or are not constant, are issues worth addressing. Individual  $\phi_{ij}$  can take values somewhat larger than unity, provided that the  $\{\bar{\phi}_i\}$  are positive (the same is true when the  $C_i T_i$  are not all equal, requiring that the  $\{\Gamma_i\}$  be positive, a condition which will depend upon the values of the  $C_i T_i$  themselves). Negative  $\phi$  do not appear to violate any of the constraints, suggesting that cases where group interactions are controlled by *disaffinity* or avoidance are permissible. The proper necessary and sufficient constraint on the values of the  $\phi$  is given by the restriction to positivity for the  $p_{ij}$ . As a result, the range of  $\phi_{ij}$  for which solutions may be obtained will

vary between dynamic models (in which the mixing process is embedded), and probably with time within any given model, but this range will always include  $[0,1]$ . Hence although we cannot easily give explicit general numerical ranges for the  $\phi$ , we have this guaranteed sub-range.

A further sufficient condition for the range of the  $\phi$  may be found as follows. Let  $L$  and  $U$  be lower and upper bounds on the  $\phi$ , with  $1 \geq U > L$ . Then  $1 - U < \Gamma_i < 1 - L$  (all  $i$ ), and  $1 - U < \Lambda < 1 - L$ . As  $L < \phi_{ij} < U$ , then for positivity of the  $p$  we require that  $L$  and  $U$  satisfy

$$\frac{(1 - U)^2}{1 - L} + L > 0.$$

For a given upper bound  $U$ , for example, a sufficient condition for the  $p$  to be positive is

$$L > \frac{1}{2} \left\{ 1 - \sqrt{1 + 4(1 - U)^2} \right\}.$$

With  $U = 1$ , this reduces to  $1 \geq \phi_{ij} > 0$ , while for  $U$  less than about  $-4$  we have approximately that  $U \geq \phi_{ij} > U - \frac{1}{2}$ . In what follows we shall refer to the *sufficient range*  $\phi_{ij} \in [L, U]$ , with the understanding that  $L$  and  $U$  satisfy the above constraint. Within this sufficient range, the  $\phi_{ij}$  can be constants. It should be borne in mind that constant- $\phi_{ij}$  solutions outside the sufficient range are possible; we will refer to this larger range as the *model-independent* range of constant  $\phi_{ij}$ . We have not yet established necessary and sufficient conditions for the range of the model-independent constant  $\phi$ .

There is also a *model-dependent*, extended range of  $\phi_{ij}$ , where the  $\phi_{ij}$  cannot be constants, but where suitable time- or density-dependent functions can be used. The extended range is explicitly bounded by the positivity constraint on the  $p$ ; in a static model (all  $C_i$  and  $T_i$  remain constant) it is perfectly possible to delimit the extended range, but in a dynamic model the bounds on the  $\phi$  change with time, and so constant  $\phi$  cannot be used in this range of values. An excellent example is of preferred mixing in the homosexual model of Section 2.1, where we write  $\phi_{ii} \equiv f_i / \bar{p}_i$  if  $i = j$ , zero elsewhere (the  $f_i \in (0,1)$  are a set of constants); clearly, for some dynamic models the  $\phi_{ij}$  may become unbounded. With this formulation the  $\phi$  are continuously adjusted so as to maintain a fixed proportion of contacts within one's group, *regardless* of the dynamics.

How serious a restriction on analysis the exclusive use of the  $[0,1]$  basic range for the  $\phi$  may be is still a subject of investigation. In particular, it is not yet known how great a sub-set of possible mixing

patterns may be described using constant  $\phi$  in this range.

### 3.2 Mixing and the $\phi$ .

Particularly for  $\phi$  in the basic range  $[0,1]$ , we can gain insight into the way the representation apportioned partnerships among groups. For  $N$  interacting homosexual groups under the conditions of Section 2.1 where any pair of groups may interact consider an individual from subgroup  $i$ , with partnership acquisition rate  $C_i$  per unit time. Eqs (1)–(3) and (8)–(10) imply that  $p_{ij} \geq \bar{p}_j \phi_{ij}$ . Thus, an average individual in sub-group  $i$  forms partnerships with individuals from sub-group  $j$  at the minimum rate  $C_i \phi_{ij} \bar{p}_j$ . Consequently, summing over all sub-groups, we conclude that a typical member of the  $i^{\text{th}}$  sub-group has formed partnerships (with all sub-groups) at the minimal rate of

$$C_i \sum_{k=1}^N \phi_{ik} \bar{p}_k = C_i (1 - R_i). \quad (39)$$

The remaining rates  $C_i R_i$  ( $i = 1, \dots, N$ ) will be distributed in the following manner.

Consider an  $N$ -group population, where the size of the  $j^{\text{th}}$  sub-group is  $T_j$ , where individuals form partnerships at the reduced rate  $C_j R_j$ . Assume proportionate mixing among the sub-groups in this “new” population (same population but with reduced rates for pairing). Then an average individual from subgroup  $i$ , mixing at random, forms partnerships with individuals from subgroup  $j$  at the rate

$$C_i R_i \frac{C_j R_j T_j}{\sum_{k=1}^N C_k T_k R_k} = \frac{C_i R_i R_j \bar{p}_j}{\sum_{k=1}^N \bar{p}_k R_k} \quad (40)$$

partnerships per unit time. Adding the minimal rate  $C_i \phi_{ij} \bar{p}_j$  from Eq (4), we see that a typical individual from subgroup  $i$  has formed partnerships with members of group  $j$  at the rate

$$C_i \left[ \phi_{ij} \bar{p}_j + \frac{R_i R_j \bar{p}_j}{\sum_{k=1}^N \bar{p}_k R_k} \right] = C_i \bar{p}_j \left[ \frac{R_i R_j}{\sum_{k=1}^N \bar{p}_k R_k} + \phi_{ij} \right] = C_i p_{ij}. \quad (41)$$

In the above we have made no assumption about the  $\{\phi_{ij}\}$ . They could in fact be density or frequency dependent, or even *explicitly* time dependent (we return to this point in the discussion).

For  $\phi$  in the particular sub-range  $[0,1]$ , mixing may be interpreted *as if* each group (say the  $i^{\text{th}}$ ) reserves a fraction of the rate of pair formation for interactions with the  $j^{\text{th}}$  sub-group. This fraction is the product of  $\phi_{ij}$ , which we choose to interpret as a measure of affinity, and  $\bar{p}_j$ , a measure of relative availability of partners (Eq (4)). The remainder of the rate of pair formation may then be thought of as being distributed at random (proportionate mixing) among the various sub-groups, which are now mixing at a reduced rate  $C_i R_i$ . In fact the above description holds true even for  $\phi$  which are not constant (*e.g.* functions of the  $\bar{p}_i$ , as in preferred mixing [9]), or are negative [40], so long as all the products  $C_i \phi_{ij} \bar{p}_j$  (all  $i$  and  $j$ ) remain finite.

Overall, we feel that the results of this section provide sufficient justification for us to label the  $\phi$  as inter-group affinities. There are many questions to be answered concerning the way in which STD dynamics are actually affected by the details of the  $\phi$  structure, but now that the criteria for constructing valid mixing functions for arbitrarily connected groups (Eqs (32) – (36)) is available, it should be possible to address these questions in a systematic manner. Issues related to the representation itself include the range of mixing functions available with the basic range for  $\phi$ , the formulation of realistic models where  $\phi$  depends on model variables (*e.g.* group population sizes), and analytic techniques to exploit the generality of the result in the investigation of model behavior. For example, is it possible to address questions such as; can mixing alone ever cause stability changes in a given model or class of models?.

#### 4. DISCUSSION.

There are now many mixing functions available in the literature, which allow non-random mixing between population groups to be investigated [3,8,9,15,24,27-30,34-37,46,47]. Each of these encapsulates one or more hypotheses about social or sexual behavior, and has its own set of parameters. Despite some useful recent results [19,31,48] the analysis of STD models with non-random mixing is still often a time-consuming affair, and the comparison of models (comparison of hypotheses) a labor-



ious process. Where we see the main advantage of having a mixing representation such as that discussed in this paper, is that we may in principle thereby analyze all possible mixing functions for each STD model, for any  $\mathbf{p}$  satisfying the axiomatic description of mixing may by definition be represented in a common form. In addition, with this framework it becomes extremely simple to formulate contact and pair-formation models, with the added advantage that their dynamic behavior can be compared in a straightforward manner. Both models use the same parameters and pair-formation models will reduce to contact models as the dissolution or “divorce” rate approaches infinity.

A general analysis of a model that incorporates all forms of mixing is, however not at present feasible, because the full range of behavior of  $\mathbf{p}$  when  $\phi$  is implicitly or implicitly time-dependent has not yet been evaluated. The interpretation of the  $\phi$  as inter-group affinities is an important feature, for it is then possible *by hypothesis* to treat the case of constant  $\phi$  not just as another particular mixing model, but as a characterization of an entire class of such models where affinities do not vary over the time-scale of interest. The results of Section 2.3 on the arbitrarily connected groups case are particularly encouraging in this respect, as they show that constant- $\phi$  solutions may always be obtained, even for very complicated social/sexual structures. Also, if the affinities remain constant (or approximately so), they may be estimated from data on sexual mixing. Mixing functions  $\mathbf{p}$  are not trivial to estimate, particularly as out-mixing, with groups of unknown size not included in the original study, can be a large source of error. Given a suitable survey design and appropriate statistical techniques however, these problems can be overcome, and estimates of  $\mathbf{p}$  obtained [45]. Multiple estimates, either as simultaneous replicates or as a time sequence, are required in order to estimate all the elements of  $\phi$  rigorously, but approximations may be obtained and hypothesized parametric forms for  $\phi$  fitted even from a single  $\mathbf{p}$  matrix [10,12].

Non-constant  $\phi$  raise some interesting questions: *e.g.* what may the  $\phi$  be dependent upon? The possibilities include all the variables of the STD model in which the mixing description is embedded, and not just the group sizes and activities which specify  $\bar{\mathbf{p}}$ , but must preclude the  $\mathbf{p}$  themselves, as the representation is not an implicit function. The explicit use of time  $t$  is also a possibility, for example if affinities were seasonal. Hypotheses about affinities which allow us to write the  $\phi$  as functions only of the  $\bar{\mathbf{p}}$  seem promising for analysis, as we may be able to establish general results based on consideration of the quantities  $\{\partial p_{ij} / \partial \bar{p}_k\}$ , which could then be used in the analysis of the overall STD model. It may be most convenient to calculate the  $\phi$  in terms of a hopefully small number of “control

variables" specified by differential equations. Further information on the nature of the  $\phi$  may be obtained from a number of sources. A particularly promising possibility is the use of stochastic simulations, where interactions are individual-based and explicit probabilistic rules for pair formation are used. Comparison between the  $p$  produced by such models and the deterministic representation of  $p$  should allow us to establish how affinity in the latter relates to non-random partner selection in the former. Preliminary work with such simulations suggests that some stochastic partner selection rules lead to  $p$  with an interesting and well-defined structure (Fig 1), and it is hoped that information on the structure of  $\phi$  may be forthcoming from analysis of such results. We may also be able to extract further information on the  $\phi$  by examining the equivalent  $\phi$ -structure for models not written explicitly in that form; a number of such equivalent  $\phi$  have been found [9].

### ACKNOWLEDGEMENTS

This research has been partially supported by NSF grant DMS-8906580, NIAID Grant R01 A129178-02, and Hatch project grant NYC 151-409, USDA to CC-C. SPB's research has been partially supported by funds from the office the dean of the College of Agriculture and Life Sciences, and the Mathematical Sciences Institute at Cornell University. This research is being, in part, conducted at the Cornell National Supercomputer Facility, the Center for the Theory of Simulation in Science and Engineering, which is funded in part, by the National Science Foundation, New York State, and the IBM Corporation. SPB would like to thank the participants at the Skökloster Workshop 1990 for many stimulating conversations, especially K. Hadeler, M. Morris and G. Scalia-Tomba. We also thank Graham Medley, Simon A. Levin, and two anonymous referees for their valuable comments on an earlier version of this paper.

# APPENDIX: A Gonorrhea Model.

Consider a population of sexually active heterosexual individuals divided into sub-populations by such factors as sex, race, socio-economic background, and average degree of sexual activity. We do not consider factors such as chronological age, age of infection, variable infectivity, and partnership duration. Fig (2) is a schematic of the main features of the model. There are  $N^f$  female and  $N^m$  male sub-populations, each divided into two epidemiological classes for single individuals:  $f_j(t)$  and  $m_i(t)$  (single susceptible females and males, at time  $t$ ), and  $F_j(t)$  and  $M_i(t)$  (single infected females and males), all for  $j = 1, \dots, N^f$  and  $i = 1, \dots, N^m$ . Hence the sexually active single individuals of each sex and each sub-population are given by  $T_j^f = f_j + F_j$  and  $T_i^m = m_i + M_i$ . The epidemiological classes for pairs are given by  $\pi_{ji}^{fm}$ ,  $\pi_{ji}^{Fm}$ ,  $\pi_{ji}^{fM}$ ,  $\pi_{ji}^{FM}$ , which are respectively the *numbers of pairs* of *f-with-m*, *F-with-m*, *f-with-M*, and *F-with-M* individuals. Naturally, transmission can only occur among those individuals in pair types  $\pi_{ji}^{Fm}$  or  $\pi_{ji}^{fM}$ . Note that  $\pi_{ji}^{fM} = \pi_{ij}^{Mf}$ , so that we need only consider four types of pairs. The transmission probability per unit time is constant within each pair containing one infected individual. Let  $\delta_M$  and  $\delta_F$  be the rates for male-to-female and female-to-male transmission, respectively. The *per capita* recovery rates are  $\gamma_M$  and  $\gamma_F$  for infected males and infected females, respectively, when their partner is uninfected. When both partners are infected (*F-with-M* pairs), simultaneous treatment of both is the norm for gonorrhea, so we incorporate “combined” recovery rate  $\gamma_{FM}$ , with both parties moving directly to the *f-with-m* (no infection) pair type. The *per capita* dissolution rates are  $\sigma_{fm}$ ,  $\sigma_{fM}$ ,  $\sigma_{Fm}$ , and  $\sigma_{FM}$  for the different types of pairs, and the *per capita* removal rates from sexual activity due to death or other causes are  $\mu_f$  and  $\mu_m$  for all females and all males respectively. Let  $\Lambda_j^f$  and  $\Lambda_i^m$  denote the “recruitment” rates (assumed constant) of single (assumed uninfected) individuals in the female and male populations respectively. We use the notation

$$p_{ji}^{xm} \equiv \frac{m_i}{M_i + m_i} p_{ji}^f, \quad p_{ji}^{xM} \equiv \frac{M_i}{M_i + m_i} p_{ji}^f, \quad p_{ij}^{yf} \equiv \frac{f_i}{F_i + f_i} p_{ij}^m, \quad p_{ij}^{yF} \equiv \frac{F_i}{F_i + f_i} p_{ij}^m,$$

( $x = f$  or  $F$  and  $y = m$  or  $M$ , for  $i = 1, \dots, N^m$  and  $j = 1, \dots, N^f$ ) for the fraction of pair-formations between the specified sub-groups ( $i$  and  $j$ ) which are of given infection status; for example,  $p_{ji}^{fm}$  and  $p_{ji}^{fM}$  give the fractions involving uninfected ( $m_i$ ) and infected ( $M_i$ ) males respectively. Then the gonorrhea pair formation/dissolution model is

$$\begin{aligned}
\frac{df_j}{dt} &= \Lambda_j^f + \gamma_F F_j + [\mu_M + \sigma_{fM}] \sum_{i=1}^{N^m} \pi_{ji}^{fM} + [\mu_m + \sigma_{fm}] \sum_{i=1}^{N^m} \pi_{ji}^{fm} - [C_j^f(t) + \mu_f] f_j \\
\frac{dF_j}{dt} &= [\mu_m + \sigma_{fM}] \sum_{i=1}^{N^m} \pi_{ji}^{fM} + [\mu_m + \sigma_{FM}] \sum_{i=1}^{N^m} \pi_{ji}^{FM} - [C_j^f(t) + \gamma_F + \mu_f] F_j \\
\frac{dm_i}{dt} &= \Lambda_i^m + \gamma_M M_i + [\mu_f + \sigma_{fM}] \sum_{j=1}^{N^f} \pi_{ji}^{fM} + [\mu_f + \sigma_{fm}] \sum_{j=1}^{N^f} \pi_{ji}^{fm} - [C_i^m(t) + \mu_m] m_i \\
\frac{dM_i}{dt} &= [\mu_f + \sigma_{fM}] \sum_{j=1}^{N^f} \pi_{ji}^{fM} + [\mu_f + \sigma_{FM}] \sum_{j=1}^{N^f} \pi_{ji}^{FM} - [C_i^m(t) + \gamma_M + \mu_m] M_i \\
\frac{d\pi_{ji}^{fm}}{dt} &= C_j^f(t) p_{ji}^{fm} f_j + \gamma_M \pi_{ji}^{fM} + \gamma_F \pi_{ji}^{FM} + \gamma_{FM} \pi_{ji}^{FM} - [\mu_f + \mu_m + \sigma_{fm}] \pi_{ji}^{fm} \\
\frac{d\pi_{ji}^{Fm}}{dt} &= C_j^f(t) p_{ji}^{Fm} F_j + \gamma_M \pi_{ji}^{FM} - [\mu_f + \mu_m + \sigma_{Fm} + \delta_F + \gamma_F] \pi_{ji}^{Fm} \\
\frac{d\pi_{ji}^{fM}}{dt} &= C_j^f(t) p_{ji}^{fM} f_j + \gamma_F \pi_{ji}^{FM} - [\mu_f + \mu_m + \sigma_{fM} + \delta_M + \gamma_M] \pi_{ji}^{fM} \\
\frac{d\pi_{ji}^{FM}}{dt} &= C_j^f(t) p_{ji}^{FM} F_j + \delta_F \pi_{ji}^{Fm} + \delta_M \pi_{ji}^{fM} - [\mu_f + \mu_m + \sigma_{FM} + \gamma_M + \gamma_F + \gamma_{FM}] \pi_{ji}^{FM}
\end{aligned}$$

with initial conditions  $f_j(0) > 0$ ,  $m_i(0) > 0$ ,  $\pi_{ji}^{fm}(0) > 0$ ,  $\pi_{ji}^{fM}(0) = 0$ ,  $\pi_{ji}^{Fm}(0) = 0$ ,  $\pi_{ji}^{FM}(0) = 0$ , and at least one of the  $F_j(0)$  and  $M_i(0)$  greater than zero (for  $i = 1, \dots, N^m$  and  $j = 1, \dots, N^f$ ).

Only the female activity levels  $C^f(t)$  appear explicitly in the equations for numbers of pairs; this is a consequence of Eq (13). Constraint (23) requires that some or all of the group-activity levels must be adjusted at each time  $t$  in order for a solution to the mixing problem to exist. As an example of a procedure for maintaining (23), we use a somewhat complicated scheme whereby both males and females have “target” levels of activity ( $\hat{C}^f$  and  $\hat{C}^m$ , respectively; these need not be constants), with their true levels calculated in terms of hypothetical rules. In particular, we assume a parameter describing the degree of female choice;  $0 < \delta < 1$ :  $\delta = 1$  implies females achieve their target and males adjust, while  $\delta = 0$  implies the converse. Let  $\kappa_j^f(t)$  and  $\kappa_i^m(t)$  be the values of partner acquisition rates for the female and male groups, respectively, which would occur when males and females (respectively) get to dominate the choice of number of partners. Then we may approximate the group acquisition

rates by

$$C_j^f(t) = \delta \hat{C}_j^f + (1 - \delta) \kappa_j^f(t) \quad , \quad C_i^m(t) = (1 - \delta) \hat{C}_i + \delta \kappa_i^m(t)$$

( $j = 1, \dots, N^f$ ,  $i = 1, \dots, N^m$ ). We use a hypothetical scheme where the  $\kappa$ 's are proportional to the level of affinity or preference for the group in the other sex's population, and inversely proportional to the representation of its group in the home sex population. The implication is that "popular" groups tend to have higher acquisition rates, and that being scarce increases the rate for *individuals* in any group. We define

$$n_i^m(t) = \frac{T_j^m(t)}{\sum_{u=1}^{N^m} T_u^m(t)} \quad , \quad n_j^f(t) = \frac{T_j^f(t)}{\sum_{v=1}^{N^f} T_v^f(t)}$$

as the fractional contributions of particular groups to the population of the same sex, and

$$\bar{\phi}_i^m(t) = \sum_{v=1}^{N^f} n_v^f(t) \phi_{vi}^f \quad , \quad \bar{\phi}_j^f(t) = \sum_{u=1}^{N^m} n_u^m(t) \phi_{uj}^m$$

as the average affinity or preference levels for each group, weighted with respect to all the groups of the other sex. Then we have

$$\kappa_i^m(t) = \frac{1}{T_i^m(t)} \frac{\bar{\phi}_i^m(t)}{\sum_{u=1}^{N^m} \bar{\phi}_u^m(t)} \sum_{v=1}^{N^f} \hat{C}_v^f(t) T_v^f(t) \quad , \quad \kappa_j^f(t) = \frac{1}{T_j^f(t)} \frac{\bar{\phi}_j^f(t)}{\sum_{v=1}^{N^f} \bar{\phi}_v^f(t)} \sum_{u=1}^{N^m} \hat{C}_u^m(t) T_u^m(t)$$

Given a particular choice of  $\phi$ , the mixing/gonorrhea problem is now fully specified. There are of course any number of schemes for calculating the activity levels; the choice must depend on the modeler's beliefs concerning behavior in the system under study. The equivalent age-structured model may be found in [16].

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**FIGURE CAPTIONS**

**Figure 1.**

Results of stochastic simulations with two sexes. Probability of two individuals who meet forming a pair is proportional to  $1 - 1 / \left( 1 + Q (|\gamma_a - \gamma_b|)^{-1} \right)$ , where the  $\{\gamma_x\}$  are the numbers of sexual partners to date for each individual, and  $Q$  measures sensitivity to the difference in experience of prospective partners (small  $Q$  implies strong preference for a partner of similar experience). Curve is of  $r$ , the correlation coefficient associated with the surface  $\mathbf{p}$  generated by each simulation. Note the approximate scaling region where  $r \propto -\log_{10}(Q)$ . Each point on the curve represents  $10^2$  replicate simulations with  $10^3$  individuals in each.

**Figure 2.**

Schematic outline of the pair formation/dissolution gonorrhea model of the appendix. Key:  $f$  = single uninfected females,  $F$  = single infected females,  $m$  = single uninfected males,  $M$  = single infected males,  $fm$  = uninfected pair,  $fM$  = uninfected female and infected male in pair,  $Fm$  = infected female and uninfected male in pair,  $FM$  = both partners infected in pair.

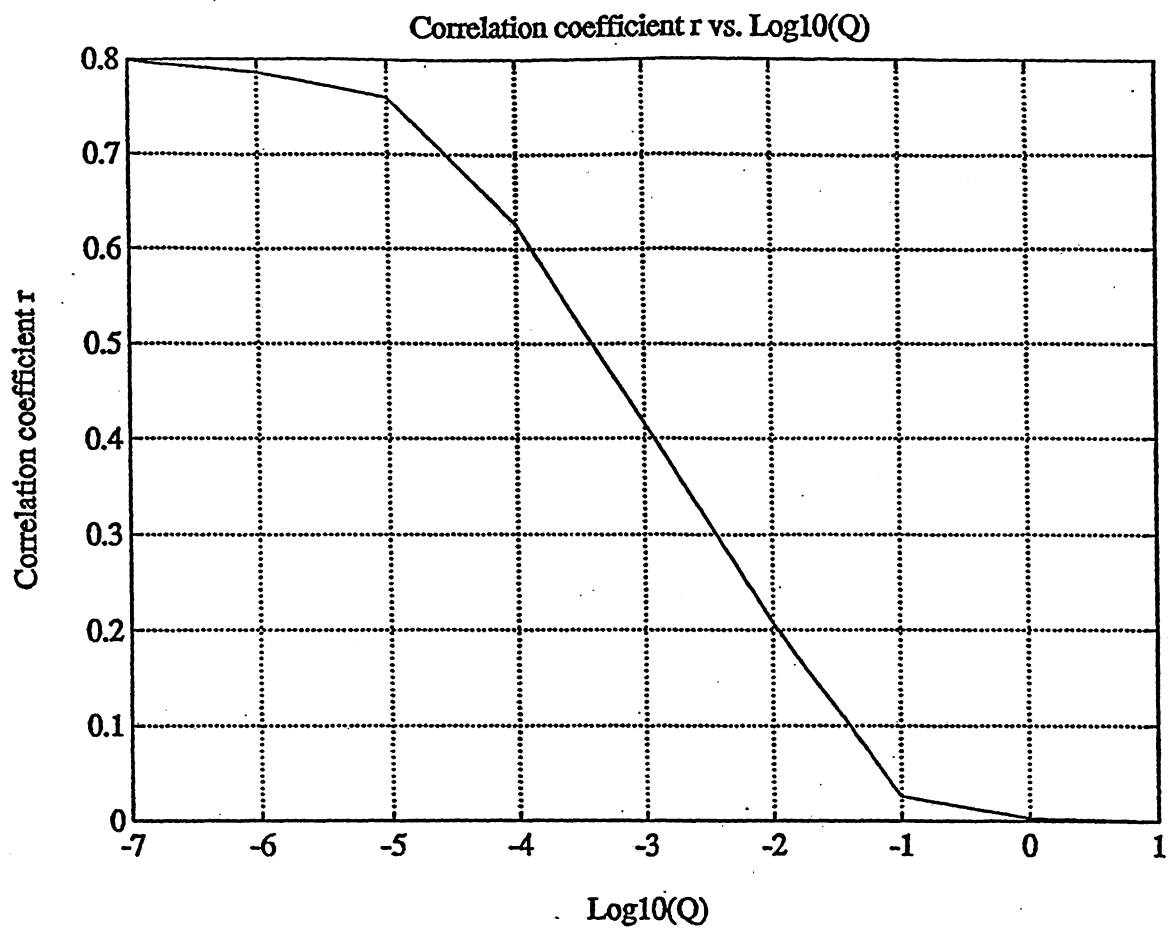


Fig 1

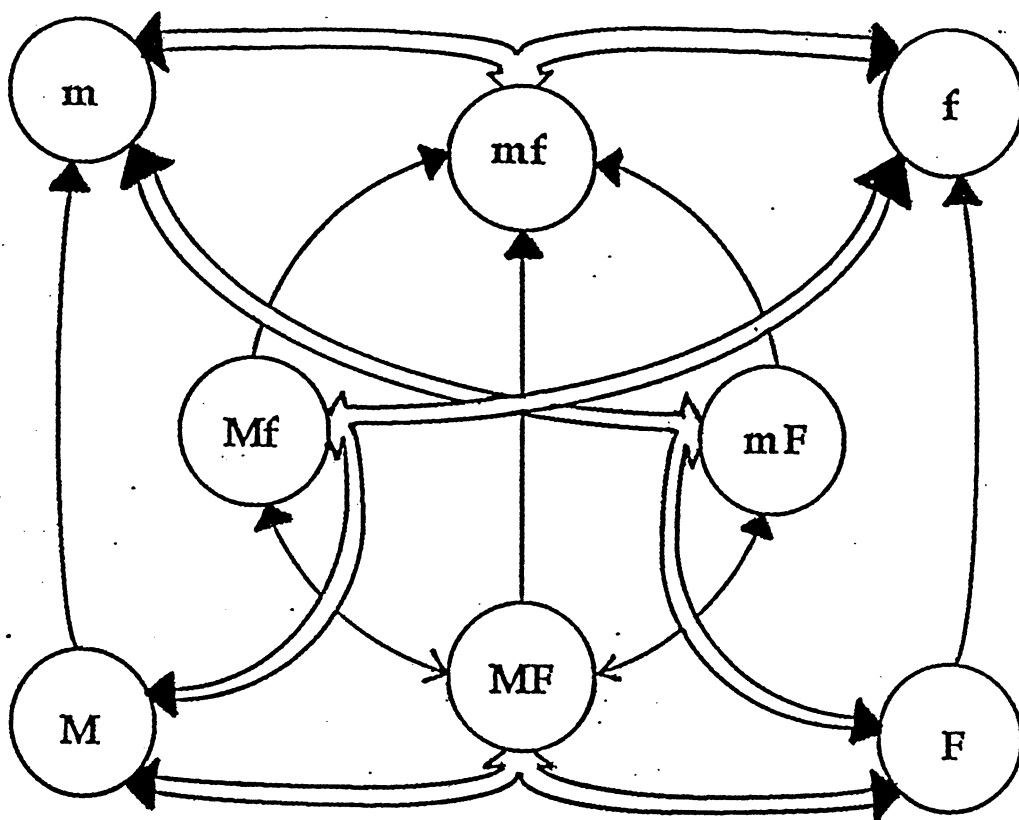


FIG 2